## Benchmark for Reactive Multiphase Flow in Porous Media Full results

Etienne Ahusborde, Brahim Amaziane, Stephan deHoop, Mustapha El Ossmani, Eric Flauraud, François P. Hamon, Michel Kern, Adrien Socié, Danyang Su, K. Ulrich Mayer, Michal Tóth and Denis Voskov

### September 5, 2023

#### Contents

1	Test 1.1: 1D kinetic chemistry	2
<b>2</b>	Test 1.2: 1D equilibrium chemistry	4
3	Test 2.1: 2D without gravity	6
	3.1 Contour maps for the Test 2.1 without gravity	. 6
	3.2 Vertical line at $x = 40$ m for the Test 2.1 without gravity	. 9
	3.3 Horizontal line at $y = 50$ m for the Test 2.1 without gravity	. 10
4	Test 2.1 : 2D with gravity	11
	4.1 Contour maps for the Test 2.1 with gravity	. 11
	4.2 Vertical line at $x = 40$ m for the Test 2.1 with gravity	. 14
	4.3 Horizontal line at $y=50$ m for the Test 2.1 with gravity	. 15
5	Test 2.2: 2D extended chemical system	16
	5.1 Contour maps for Test 2.2	. 16
	5.2 Vertical line at $x = 40$ m for the Test 2.2	
	5.3 Horizontal line at $y = 50$ m for the Test 2.2	. 19

### 1 Test 1.1: 1D kinetic chemistry

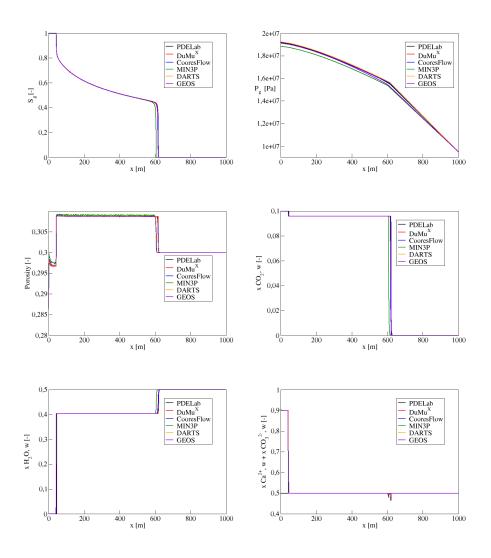


Figure 1: Comparison of gas saturation (top left), gas pressure (top right), porosity (middle left), liquid  $CO_2$  fraction (middle right), liquid water fraction (bottom left), liquid total ion fraction (bottom right) at t=1000 days for Test 1.1.

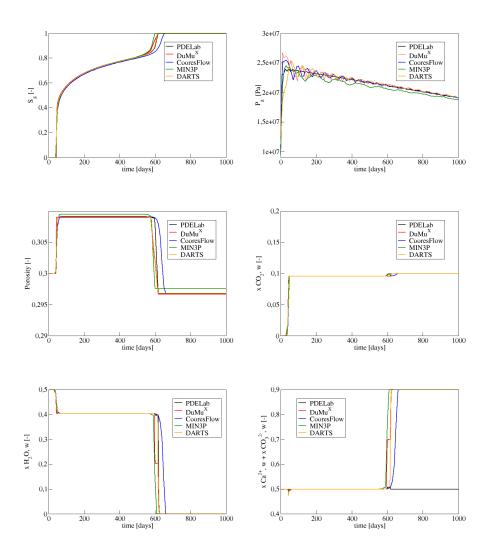


Figure 2: Comparison of gas saturation (top left), gas pressure (top right), porosity (middle left), liquid  $CO_2$  fraction (middle right), liquid water fraction (bottom left), liquid total ion fraction (bottom right) at x=25 m for Test 1.1.

### 2 Test 1.2: 1D equilibrium chemistry

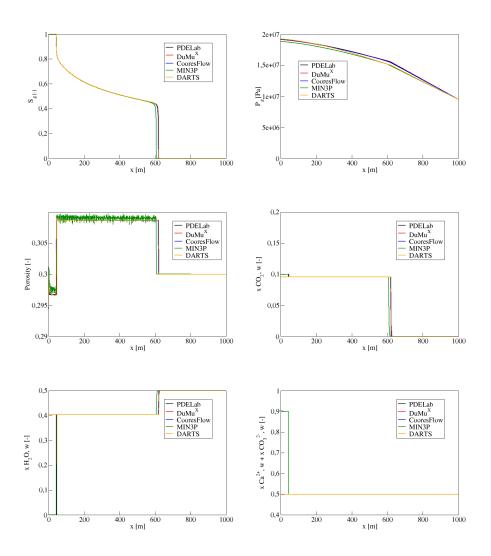


Figure 3: Comparison of gas saturation (top left), gas pressure (top right), porosity (middle left), liquid  $CO_2$  fraction (middle right), liquid water fraction (bottom left), liquid total ion fraction (bottom right) at t = 1000 days for Test 1.2.

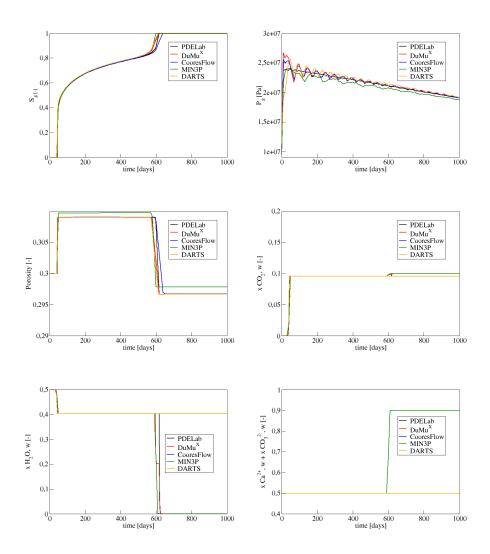


Figure 4: Comparison of gas saturation (top left), gas pressure (top right), porosity (middle left), liquid  $CO_2$  fraction (middle right), liquid water fraction (bottom left), liquid total ion fraction (bottom right) at x=25 m for Test 1.2.

### 3 Test 2.1: 2D without gravity

### 3.1 Contour maps for the Test 2.1 without gravity

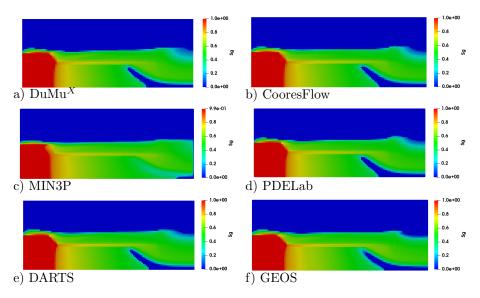


Figure 5: Comparison of gas saturation  $S_g$  at t=1000 days for Test 2.1 without gravity.

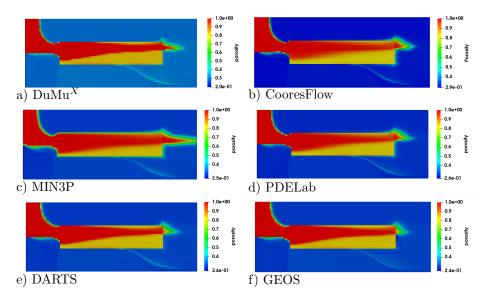


Figure 6: Comparison of porosity  $\phi$  at t=1000 days for Test 2.1 without gravity.

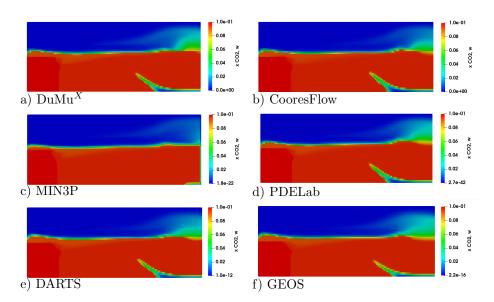


Figure 7: Comparison of liquid  ${\rm CO}_2$  fraction  $x_{CO_2,w}$  at t=1000 days for Test 2.1 without gravity.

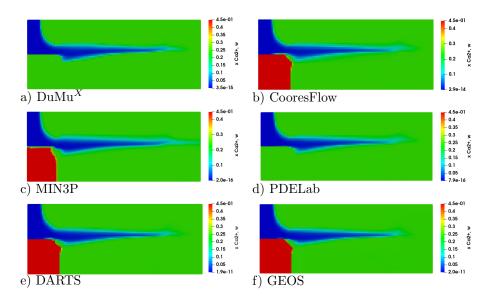


Figure 8: Comparison of liquid Ca<sup>2+</sup> fraction  $x_{Ca^{2+},w}$  at t=1000 days for Test 2.1 without gravity.

## 3.2 Vertical line at x = 40 m for the Test 2.1 without gravity

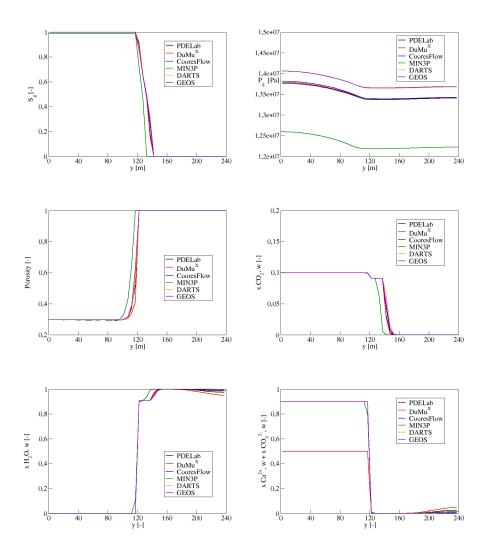


Figure 9: Comparison of gas saturation (top left), gas pressure (top right), porosity (middle left), liquid  $CO_2$  fraction (middle right), liquid water fraction (bottom left), liquid total ion fraction (bottom right) at t=1000 days on vertical line x=40 m for Test 2.1 without gravity.

## 3.3 Horizontal line at y = 50 m for the Test 2.1 without gravity

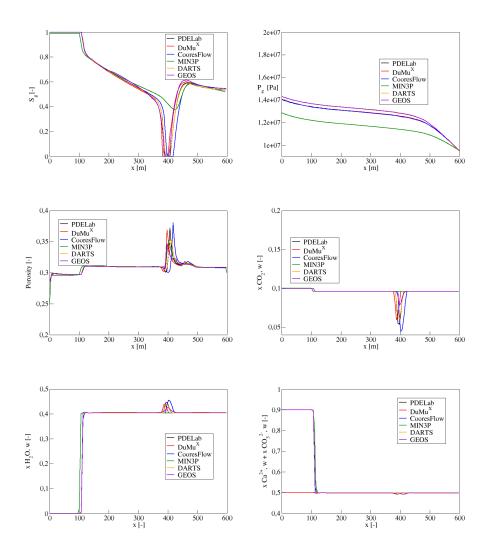


Figure 10: Comparison of gas saturation (top left), gas pressure (top right), porosity (middle left), liquid  $CO_2$  fraction (middle right), liquid water fraction (bottom left), liquid total ion fraction (bottom right) at t=1000 days on the horizontal line y=50 m for Test 2.1 without gravity.

## 4 Test 2.1 : 2D with gravity

### 4.1 Contour maps for the Test 2.1 with gravity

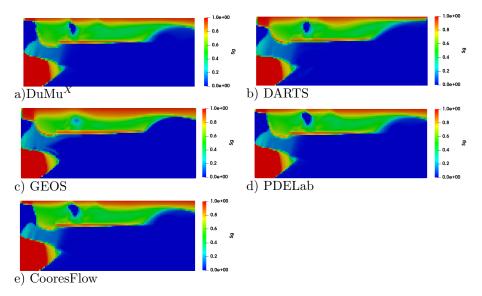


Figure 11: Comparison of gas saturation  $S_g$  at t=1000 days for the 2D test with simple chemistry and with gravity.

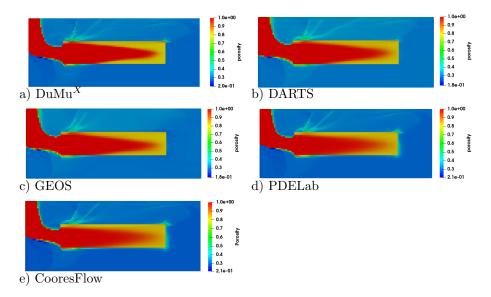


Figure 12: Comparison of porosity  $\phi$  at t=1000 days for the Test 2.1 with gravity.

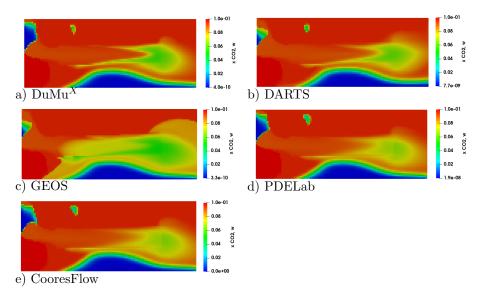


Figure 13: Comparison of liquid CO<sub>2</sub> fraction  $x_{CO_2,w}$  at t=1000 days for the Test 2.1 with gravity.

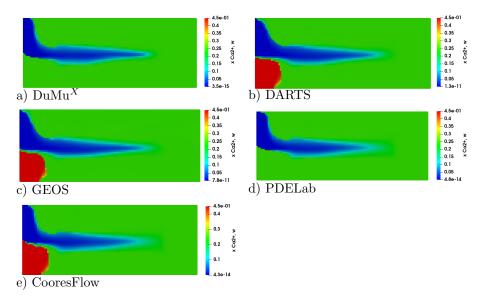


Figure 14: Comparison of liquid Ca<sup>2+</sup> fraction  $x_{Ca^{2+},w}$  at t=1000 days for the Test 2.1 with gravity.

### 4.2 Vertical line at x = 40 m for the Test 2.1 with gravity

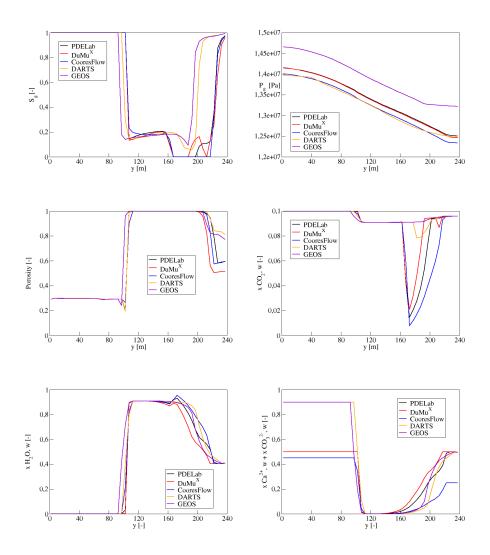


Figure 15: Comparison of gas saturation (top left), gas pressure (top right), porosity (middle left), liquid  $CO_2$  fraction (middle right), liquid water fraction (bottom left), liquid total ion fraction (bottom right) at t=1000 days on vertical line x=40 m for Test 2.1 with gravity.

# 4.3 Horizontal line at y = 50 m for the Test 2.1 with gravity

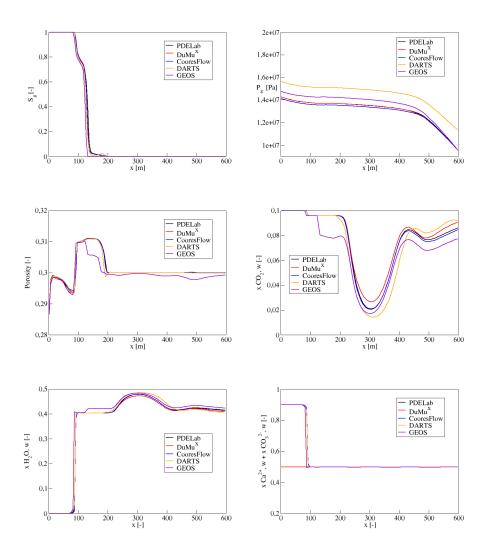


Figure 16: Comparison of gas saturation (top left), gas pressure (top right), porosity (middle left), liquid  $CO_2$  fraction (middle right), liquid water fraction (bottom left), liquid total ion fraction (bottom right) at t=1000 days on vertical line y=50 m for Test 2.1 with gravity.

### 5 Test 2.2: 2D extended chemical system

#### 5.1 Contour maps for Test 2.2

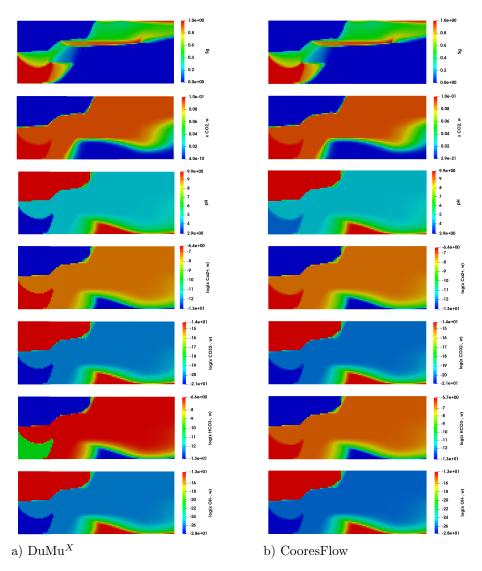


Figure 17: Comparison of several quantities at t=1000 days for the Test 2.2 (left column: DuMu<sup>X</sup>, right column: CooresFlow). From top to bottom: gas saturation, liquid CO<sub>2</sub> fraction, pH, logarithm of liquid Ca<sup>2+</sup> fraction, logarithm of CO<sub>3</sub><sup>2-</sup>, logarithm of liquid HCO<sub>3</sub><sup>-</sup> fraction, logarithm of OH<sup>-</sup>

5.2 Vertical line at x = 40 m for the Test 2.2

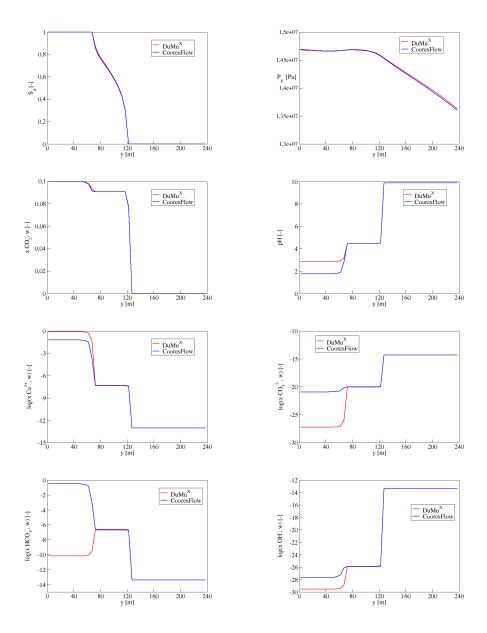


Figure 18: Comparison of gas saturation (top left), gas pressure (top right), liquid  $\mathrm{CO}_2$  fraction (second row left), pH (second row right), logarithm of liquid  $\mathrm{Ca}^{2+}$  fraction (third row left), logarithm of liquid  $\mathrm{CO}_3^{2-}$  fraction (third row right) , logarithm of  $\mathrm{HCO}_3^{-}$  (bottom left), logarithm of  $\mathrm{OH}^{-}$  (bottom right) at t=1000 days on vertical line x=40 m for Test 2.2.

5.3 Horizontal line at y = 50 m for the Test 2.2

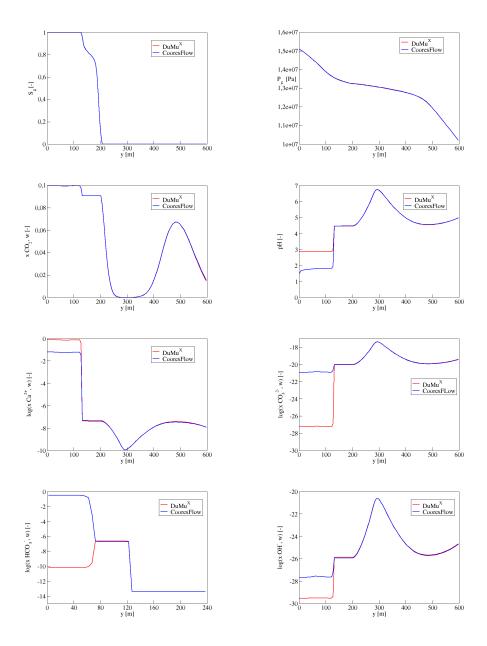


Figure 19: Comparison of gas saturation (top left), gas pressure (top right), liquid  $\mathrm{CO}_2$  fraction (second row left), pH (second row right), logarithm of liquid  $\mathrm{Ca}^{2+}$  fraction (third row left), logarithm of liquid  $\mathrm{CO}_3^{2-}$  fraction (third row right), logarithm of  $\mathrm{HCO}_3^{-}$  (bottom left), logarithm of  $\mathrm{OH}^{-}$  (bottom right) at t=1000 days on vertical line y=50 m for the Test 2.2.